

Thiamine disulfide

67-16-3 | DTXSID6046890

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

Model Results

Predicted value: 1.62e-08 mmHg

Global applicability domain: Outside

Local applicability domain index: 1.23e-01

Confidence level: 3.74e-01

Nearest Neighbors from the Training Set

| | | |
|---|---|--|
| <div>Image not found</div> <div>Ethoxysulfuron</div> <div>Measured: 1.65e-07</div> <div>Predicted: 5.60e-08</div> | <div>Image not found</div> <div>Cyprodinil</div> <div>Measured: 1.13e-08</div> <div>Predicted: 1.18e-06</div> | <div>Image not found</div> <div>9,10-Anthracenedione, 1,4-bis(methylamino)-</div> <div>Measured: 1.80e-08</div> <div>Predicted: 4.57e-11</div> |
| <div>Image not found</div> <div>Amidosulfuron</div> <div>Measured: 3.38e-10</div> <div>Predicted: 5.63e-08</div> | <div>Image not found</div> <div>1-Isobutoxypropan-2-ol</div> <div>Measured: 7.13e-08</div> <div>Predicted: 1.69</div> | |